

Nonequilibrium particle and energy currents in quantum chains connected to mesoscopic Fermi reservoirs

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We propose a model of nonequilibrium quantum transport of particles and energy in a system connected to mesoscopic Fermi reservoirs (meso-reservoir). The meso-reservoirs are in turn thermalized to prescribed temperatures and chemical potentials by a simple dissipative mechanism described by the Lindblad equation. As an example, we study transport in monoatomic and diatomic chains of non-interacting spinless fermions. We show numerically the breakdown of the Onsager reciprocity relation due to the dissipative terms of the model.

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Introduction.- Nonequilibrium systems abound in nature and still their theoretical description poses numerous challenges to theory. Nonequilibrium steady states (NESS) describe the state of a system maintained out of equilibrium by external forces such as *e.g.*, gradients of temperature T and chemical potential μ , and are characterized by the emergence of steady flows. One might expect that a finite system connected to two infinitely extended reservoirs imposing external gradients, will reach a NESS after a sufficiently long time [1, 2]. Nonetheless, this is not always the case and the conditions to reach a NESS are not well understood in general. Although the problem of existence and approach to NESS has been discussed since the early days of statistical mechanics, rigorous results are limited to a few examples [3–5], and to near equilibrium regimes. The extension to regimes beyond linear response faces the difficulty arising from infiniteness of the reservoirs [6, 7].

In quantum mechanics the construction of NESS requires to consider open quantum systems, rendering the problem extraordinarily more difficult. The common setup is to consider the infinite time limit of the density matrix of the finite system S coupled to two infinite reservoirs which are in thermal equilibrium at different temperatures and chemical potentials, starting from initial separable state $\rho_L \otimes \rho_S \otimes \rho_R$. One can then study the properties of the density operator of the total (infinite) system [1, 2], or the reduced density operator for the (finite) system S [8], obtained by tracing out the reservoirs' degrees of freedom. The time evolution of the density operator is naturally determined by the Von Neumann equation. However, dealing with infinite degrees of freedom is in most cases difficult. A second approach based on the master equation of the reduced density operator

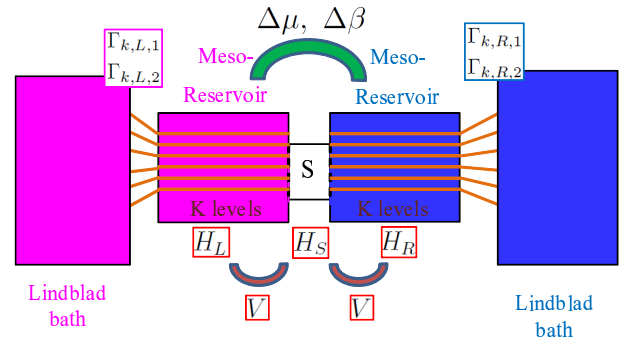


FIG. 1: (Color online) The schematic view of the two-level reservoir open system model.

is more accessible, albeit at the price of several approximations such as *e.g.*, Born-Markov (see *e.g.* [9]).

In this Letter, we propose a conceptually different approach for the study of NESS that comprises meso-reservoirs with a finite number of degrees of freedom, which in turn are thermalized by Markovian macroscopic reservoirs using a simple Lindblad equation. This setup yields a computationally efficient model in which the NESS of the system and of the meso-reservoirs are mathematically accessible, thus allowing to study characteristic features depending on the number of degrees of freedom of the meso-reservoirs, such as relaxation times of the system and of the meso-reservoirs, or correlations among them. It is interesting remarking that finite meso-reservoirs in principle allow the creation of entanglement among the different degrees of freedom of the system solely through its coupling with the meso-reservoir [10], thus making our setup much richer.

The model.- We consider a one-dimensional quantum

chain of spinless fermions coupled at its boundaries to meso-reservoirs comprising a finite number of spinless fermions with wave number k ($k \in \{1, \dots, K\}$). The Hamiltonian of the system can be written as $H = H_S + H_L + H_R + V$, where

$$\begin{aligned} H_S &= - \sum_{j=1}^{n-1} \left(t_j c_j^\dagger c_{j+1} + (\text{h.c.}) \right) + \sum_{j=1}^n U c_j^\dagger c_j, \quad (1) \\ H_\alpha &= \sum_{k=1}^K \epsilon_k a_{k\alpha}^\dagger a_{k\alpha}, \quad \epsilon_k \equiv \theta_F(k - k_0), \quad \alpha = \{L, R\} \\ V &= \sum_{k=1}^K v \left(a_{kL}^\dagger c_1 + a_{kR}^\dagger c_n \right) + (\text{h.c.}), \end{aligned}$$

and where $\{t_j\}$ are the nearest neighbor hoppings, U is the onsite potential, v is the coupling between the system and the meso-reservoirs, and c_j, c_j^\dagger is the annihilation/creation operator for the spinless fermions of the chain, while $a_{k,\alpha}, a_{k,\alpha}^\dagger$ are that of the left and right meso-reservoirs.

The key idea of our model is to enforce the finite meso-reservoirs to equilibrium using simple Lindblad dissipators [11–13]. If the couplings to the Lindblad dissipators are small, then we can interpret these terms as coming from tracing out infinitely extended (super-)reservoirs (schematically depicted in Fig. 1). Thus, the density matrix of the total setup evolves according to the many-body Lindblad equation

$$\begin{aligned} \frac{d}{dt} \rho &= -i[H, \rho] \quad (2) \\ &+ \sum_{k,\alpha,m} \left(2L_{k,\alpha,m} \rho L_{k,\alpha,m}^\dagger - \{L_{k,\alpha,m}^\dagger L_{k,\alpha,m}, \rho\} \right) \\ L_{k,\alpha,1} &= \sqrt{\Gamma_{k,\alpha,1}} a_{k\alpha}, \quad L_{k,\alpha,2} = \sqrt{\Gamma_{k,\alpha,2}} a_{k\alpha}^\dagger \\ \Gamma_{k,\alpha,1} &= \gamma(1 - F_\alpha(\epsilon_k)), \quad \Gamma_{k,\alpha,2} = \gamma F_\alpha(\epsilon_k), \end{aligned}$$

where $L_{k,\alpha,1}$ and $L_{k,\alpha,2}$ are operators representing the coupling to the super-reservoirs, $F_\alpha(\epsilon) = (e^{\beta_\alpha(\epsilon - \mu_\alpha)} + 1)^{-1}$ are Fermi distributions, with inverse temperatures β_α and chemical potentials μ_α , and $[\cdot, \cdot]$ and $\{\cdot, \cdot\}$ denote the commutator and anti-commutator, respectively. Generalization to spinfull fermions (e.g. electrons) is straightforward. The parameter γ determines the strength of the coupling to the super-reservoirs and, as we shall show later, needs to be fine-tuned in order to ensure the applicability of the model. We note that the parameter γ determining the rate of relaxation of the meso-reservoirs to equilibrium, in general can depend on temperature, chemical potential, and wave-number k of the meso-reservoir modes. Here we consider the simplest model possible and take γ as constant. We stress that our model does not rely on the usual weak-coupling assumption needed for the physical derivation of the Lindblad master equation [8], thus γ does not need to be a small parameter.

Results.— We have studied monoatomic ($t_j = t$) and diatomic ($t_{2j-1} = t_A, t_{2j} = t_B$) chains. Unless specified differently, we have set $\gamma = 0.1$, $v = 0.03$, $\epsilon_1 = -20$, $\epsilon_K = 20$, $K = 200$, $t = 3$, and $\mu_L = -\mu_R = \mu$.

When the system and the meso-reservoirs are decoupled ($v = 0$), each non-interacting mode of the meso-reservoir is thermalized separately with the prescribed Fermi-Dirac occupation number [14]. For small v , $v \ll \gamma$, we thus expect the distribution of occupations in the meso-reservoirs to be close to Fermi-Dirac, as shown in Fig. 2(a). A remarkable feature of our model is that we can monitor and control the difference of occupation distributions $\langle a_{k\alpha}^\dagger a_{k\alpha} \rangle - F_\alpha(\epsilon_k)$ by changing the coupling parameters v or γ . Here and below $\langle \cdot \rangle$ represents an expectation value with respect to the NESS.

Looking at the occupation density inside the system we observe that $\langle c_j^\dagger c_j \rangle$ is almost a constant, i.e. independent of j , except at the edge of the chain, indicating that ballistic transport is expected.

We now discuss the relaxation times of the system. As shown in [15], the spectrum of the evolution superoperator is given in terms of the eigenvalues β_j (so-called rapidities) of the matrix X :

$$X = -\frac{i}{2} \mathbf{H} \otimes \sigma_y + \frac{\gamma}{2} \begin{pmatrix} \mathbf{E}_K & \mathbf{0}_{K \times n} & \mathbf{0}_{K \times K} \\ \mathbf{0}_{n \times K} & \mathbf{0}_{n \times n} & \mathbf{0}_{n \times K} \\ \mathbf{0}_{K \times K} & \mathbf{0}_{K \times n} & \mathbf{E}_K \end{pmatrix} \otimes \mathbf{E}_2$$

where $\mathbf{0}_{i \times j}$ and \mathbf{E}_j denote $i \times j$ zero matrix and $j \times j$ unit matrix, σ_y is the Pauli matrix, and \mathbf{H} is a matrix which defines the quadratic form of the Hamiltonian, as $H = \mathbf{d}^T \mathbf{H} \mathbf{d}$ in terms of fermionic operators $\mathbf{d}^T \equiv \{a_{1L}, \dots, a_{KL}, c_1, \dots, c_n, a_{1R}, \dots, a_{KR}\}$. Fig. 2(b) shows a typical spectrum for the monoatomic chain. Interestingly, there is a clear separation of the relaxation times into slow and fast normal modes. The number of slow modes n_s , with eigenvectors localized in the system part, is $n_s \approx 2n$, and the number of fast modes $n_f \approx 4K$, with eigenvectors localized in the meso-reservoirs.

We have not observed rapidities with zero real part, and thus according to Ref. [14, 15], there exists a unique steady state for the range of parameters used in this Letter. Next, we study the NESS averages $\langle \cdot \rangle$ of observables. The quadratic observables are given in terms of the solution of the Lyapunov equation [15]:

$$\begin{aligned} \langle w_j w_k \rangle &= \delta_{j,k} - 4i Z_{j,k} \\ w_{2j-1} &\equiv c_j + c_j^\dagger, \quad w_{2j} \equiv i(c_j - c_j^\dagger) \\ \mathbf{X}^T \mathbf{Z} + \mathbf{Z} \mathbf{X} &\equiv \mathbf{M}_i \\ \mathbf{M}_i &\equiv -\frac{i}{2} \text{diag}\{\Gamma_{1L}^-, \dots, \Gamma_{KL}^-, \mathbf{0}_{1 \times n}, \Gamma_{1R}^-, \dots, \Gamma_{KR}^-\} \otimes \sigma_y \\ \Gamma_{k\alpha}^- &\equiv \Gamma_{k,\alpha,2} - \Gamma_{k,\alpha,1} = \gamma_{k\alpha} \{2F_\alpha(\epsilon_k) - 1\}, \end{aligned}$$

whereas Wick's theorem can be used to obtain expectations of higher-order observables. Let us now discuss the deviation of occupation numbers from the Fermi distribution in the meso-reservoirs. Lindblad equation of motion

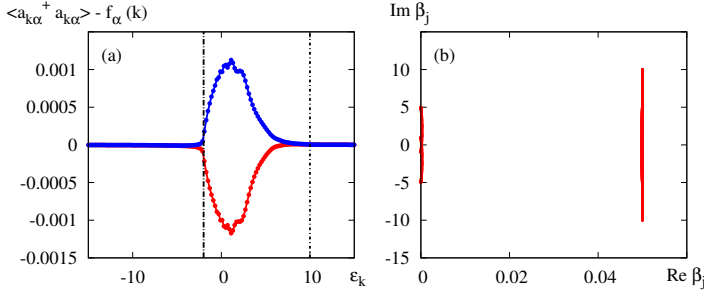


FIG. 2: (Color online) Panel (a) shows (mode) k -dependence of the deviation from the Fermi function $\langle a_{k\alpha}^\dagger a_{k\alpha} \rangle - F_\alpha(\epsilon_k)$, (red/blue curve is for the left/right meso-reservoir, and vertical lines indicate the energy band, see main text for parameter values), and Panel (b) shows the rapidity spectrum for the monoatomic chain indicating the separation of time scales.

results in the following identity, $2\gamma \left\{ \langle a_k^\dagger a_k \rangle - F_\alpha(\epsilon_k) \right\} = \langle J_k^\alpha \rangle$, where J_k^α is the k -th level contribution to the current from the α -meso-reservoir to the system, $J_k^\alpha = iv(a_{k\alpha}^\dagger c_\alpha - c_\alpha^\dagger a_{k\alpha})$ ($c_L = c_1$, $c_R \equiv c_n$). This relation can be used to determine the Lindblad dissipator from physical observables such as currents and occupation numbers. It is interesting to remark that this relation can be interpreted as a type of Landauer formula, i.e., $\langle J_{tot}^P \rangle = \sum_k 2\gamma \{ \langle a_{kL}^\dagger a_{kL} \rangle - F_L(\epsilon_k) \}$, where J_{tot}^P is the particle current from the left reservoir to the system, and shows explicitly how the nonequilibrium situation modifies the Fermi distributions. A similar expression holds for the current from the right reservoir to the system. It follows that although the distribution functions $\langle a_{k\alpha}^\dagger a_{k\alpha} \rangle$ are slightly modified by the presence of the system and the other reservoir, the integrated difference from the Fermi distribution summed over both meso-reservoirs satisfies the charge conservation, i.e., $\sum_{k,\alpha} \left\{ \langle a_{k\alpha}^\dagger a_{k\alpha} \rangle - F_\alpha(\epsilon_k) \right\} = 0$ [23].

We now turn our attention to the particle and energy currents in the system. The particle current is defined through the conservation law of number of particles:

$$\begin{aligned} \frac{dc_j^\dagger c_j}{dt} &= J_{j-1}^P - J_j^P, \quad (2 \leq j \leq n-1) \\ J_j^P &\equiv it_j(c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j), \quad (1 \leq j \leq n-1) \end{aligned}$$

and the energy current is defined through the conservation law of local energy:

$$\begin{aligned} \frac{dH_j}{dt} &= J_{j-1}^E - J_j^E, \quad (2 \leq j \leq n-1) \\ J_{j-1}^E &= i[H_{j-1}, H_j], \quad (2 \leq j \leq n) \\ H_j &\equiv t_j c_j^\dagger c_{j+1} + t_j c_{j+1}^\dagger c_j + U c_j^\dagger c_j, \quad (1 \leq j \leq n) \end{aligned}$$

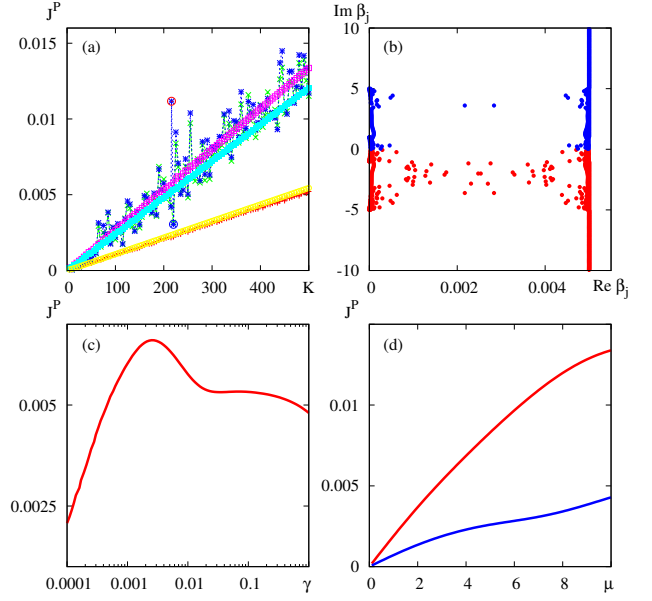


FIG. 3: (Color online) Panel (a) shows the K dependence of the particle current for the monoatomic chains (red: $\gamma = 0.0001$, green: $\gamma = 0.001$, blue: $\gamma = 0.01$, pink: $\gamma = 0.1$, cyan: $\gamma = 1$, yellow: $\gamma = 10$), and panel (b) shows the rapidities for $\gamma = 0.01$ (Using the symmetry with respect to real axis, we plot rapidities in positive/negative imaginary plane for $K = 216/K = 220$). Those two parameters are indicated in figure (a) as red ($K = 216$) and blue ($K = 220$) circles. Panel (c) shows the γ dependence of the particle current for the monoatomic chains. Panel (d) shows μ dependence of the particle current. The red line is for the monoatomic chains ($t = 3$), and the blue line is for the diatomic chains ($t_A = 3$, $t_B = 6$).

where, by definition, $c_{n+1} \equiv 0$. We have checked that both the particle and the energy current converge to a constant by increasing the system size n for the monoatomic chains. For the diatomic chains, currents converge to different constants, depending on the parity of integer n . Therefore, ballistic transport is indeed achieved.

Fig. 3(a) shows the K dependence of the particle current for the monoatomic chains with γ ranging from 0.0001 to 10. The particle current increases linearly in the number of meso-reservoir modes K , with notable fluctuations in K observed for some range of γ (which will be discussed later). We see that the particle current is roughly γ -independent for $\gamma \in [0.001, 1]$, and is somewhat smaller for very small or very large γ . The dependence on γ of the particle current, shown in Fig. 3(c), exhibits a plateau starting at $\gamma \approx v$, and one should take γ in the plateau region $[v, \|H\|]$ to have a physically meaningful model. Fig. 3(d) shows the dependence of the particle current on the bias of the chemical potential (μ). We find, as expected, initially linear increase in μ which slows down for larger μ .

The fluctuations in the current as a function of K occur because for some values of K the coupling between

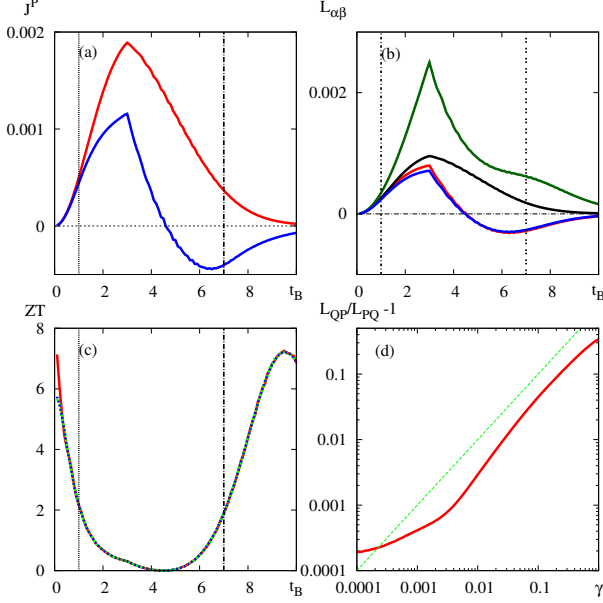


FIG. 4: (Color online) Panel (a) shows the t_B dependence of the particle current for the chains. The red line is for $\beta_L = \beta_R = 1$, and $\mu = 1$, and the blue line is for $\beta_L = 0.5$, $\beta_R = 4$, and $\mu = 0$. Panel (b) shows t_B dependence of the Onsager coefficients (color code: L_{QP} - red, L_{PP} - black, L_{QQ} - green, L_{PQ} - blue), and (c) of ZT (comparing $K = 200$ case (green) to $K = 100$ (red) and $K = 500$ (blue)), for the diatomic chains ($t_A = 3$). Chains have exponentially small current outside $t_B \in [1, 7]$ indicated in the figure. Panel (d) shows the γ dependence of asymmetry $L_{QP}/L_{PQ} - 1$ for the diatomic chain with $t_A = 3$, $t_B = 6$ (dashed line indicates linear growth). Note that asymmetry grows linearly with γ in the physical regime $\gamma > v$.

the meso-reservoirs and system is stronger. Intuitively this happens when an eigenenergy of the meso-reservoir coincides with one of the system, resulting with some eigenvector of the matrix \mathbf{X} being supported both in the system and the meso-reservoirs, breaking the separation into slow and fast modes. When the density of states of the meso-reservoir becomes dense enough such that it is smooth (average level spacing smaller than the width given by the coupling γ to the super-reservoirs), the current becomes a smooth function of K or equivalently of the density of states. These ideas are confirmed by the numerical results in Fig. 3(a,b). We note however, the current fluctuations are strong only in the ‘non-physical’ regime $\gamma < v$.

Fig. 4(a) shows the dependence of the particle current driven by either thermal or chemical gradients, on the hopping strength (t_B) for diatomic chains. Where the particle current is negative, the energy band of the chain is located entirely below the fermi energy of the cooler reservoir, yielding a particle current flow from the cold to the hot reservoir. Such crossed transport (and its counterpart of the energy current driven by the chemical gradient), can be exploited to pump heat or particles [16].

For sufficiently small thermal and chemical gradients, the particle and heat current defined as $J_Q \equiv J_E - \bar{\mu}J_P$ ($\bar{\mu} = (\mu_L + \mu_R)/2$), depend linearly on the external gradients as [17–19]

$$\begin{aligned} J_Q &= L_{QQ}\Delta\beta + L_{QP}\Delta(-\beta\mu), \\ J_P &= L_{PQ}\Delta\beta + L_{PP}\Delta(-\beta\mu), \end{aligned}$$

where $\Delta\beta \equiv \beta_R - \beta_L$ and $\Delta(\beta\mu) \equiv \beta_R\mu_R - \beta_L\mu_L$. The second law of thermodynamics imposes definiteness of the matrix of Onsager coefficients \mathbf{L} , which implies $L_{QQ} \geq 0$ and $L_{PP} \geq 0$, and if the dynamics is time-reversible, the Onsager’s reciprocity relation $L_{PQ} = L_{QP}$ holds. In Fig. 4 we consider diatomic chains with $t_A = 3$ and show the dependence of various properties of \mathbf{L} on the other hopping parameter t_B . Fig. 4(b) shows the t_B dependence of all Onsager coefficients, whereas in Fig. 4(c) shows the thermoelectric figure-of-merit $ZT \equiv L_{PQ}L_{QP}/\det\mathbf{L}$ [20]. One sees that while non-diagonal elements L_{QP} or L_{PQ} can be sometimes negative, L_{QQ} , L_{PP} are always positive. Moreover, ZT reaches large values only for disproportionate hopping rates t_A and t_B .

On the other hand, systems interacting with environments inevitably include irreversible processes, which breaking down time-reversibility invariance and thus, the validity of the Onsager reciprocity relation [21]. Fig. 4(d) shows the γ dependence of L_{PQ}/L_{QP} , and we see that the relation is roughly linearly broken by increasing γ , and thus, we conclude that the Onsager reciprocity relation is satisfied only if there is a time reversible dynamics for the total system, including the super-reservoirs, which is the case in which the Onsager reciprocity relation is rigorously proved [22]. We recall that $\gamma \ll 1$ is one of the necessary conditions for deriving the Lindblad equation, by taking a partial trace of the unitary time evolution, thus $|L_{PQ}/L_{QP} - 1|$ can be understood as an error-indicator due to the weak-coupling assumption. We remark that the transport coefficients for the diatomic chains (shown in Fig. 3(d) and Fig. 4) are non-smooth functions of t_B at the mono-atomic point $t_B = t_A$.

Conclusion.- We have introduced a model in the framework of open quantum systems with finite meso-reservoirs which nicely describes non-equilibrium steady states of quantum chains. We have checked that this model has a regime which is robust with respect to the strength of the Lindblad dissipators, and the occupation number distributions of meso-reservoirs are close to the Fermi distribution, the difference being determined by the particle current. We observed that the decay times of normal modes show a clear separation into slow and fast decaying modes. In a certain regime we find a possibility of strongly fluctuating currents (as a function of any generic parameter) which is attributed to existence of well separated intermediate (resonant) decay modes. We find possibility of negative non-diagonal elements of

the Onsager matrix but confirm the positivity of the full Onsager matrix. The Onsager reciprocal relation was shown to be correct only for weak coupling $\gamma \ll 1$, and the symmetry is broken linearly as a function of γ .

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